

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081822\
 Data File : BF129894.D
 Acq On : 19 Aug 2022 01:01
 Operator : CG\JU
 Sample : N4211-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129894.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	460	463	475	rBV	213305	268134	8.26%	1.321%
2	5.428	531	534	553	rBV	2672145	2704682	83.30%	13.329%
3	6.445	703	707	721	rBV	2956366	2714635	83.61%	13.379%
4	6.792	762	766	773	rBV	874850	761387	23.45%	3.752%
5	7.357	858	862	872	rBV	1829004	1783167	54.92%	8.788%
6	8.075	980	984	987	rBV	1162425	980134	30.19%	4.830%
7	9.151	1161	1167	1170	rBV	3584716	3246924	100.00%	16.002%
8	9.827	1277	1282	1286	rBV	1139099	985913	30.36%	4.859%
9	10.627	1414	1418	1421	rBV	1577652	1449608	44.65%	7.144%
10	11.321	1532	1536	1539	rBV	981069	795258	24.49%	3.919%
11	11.698	1596	1600	1603	rBV	63841	58217	1.79%	0.287%
12	12.410	1714	1721	1724	rBV	102207	101092	3.11%	0.498%
13	12.904	1801	1805	1809	rBV	2748979	2400507	73.93%	11.830%
14	13.798	1953	1957	1970	rBV5	60164	176686	5.44%	0.871%
15	13.968	1982	1986	1990	rBV	774164	729193	22.46%	3.594%
16	14.057	1995	2001	2007	rBV	373669	393673	12.12%	1.940%
17	15.039	2165	2168	2175	rVB3	48581	66810	2.06%	0.329%
18	15.433	2229	2235	2240	rVB	482017	631365	19.45%	3.112%
19	15.833	2300	2303	2308	rVB2	33704	43574	1.34%	0.215%

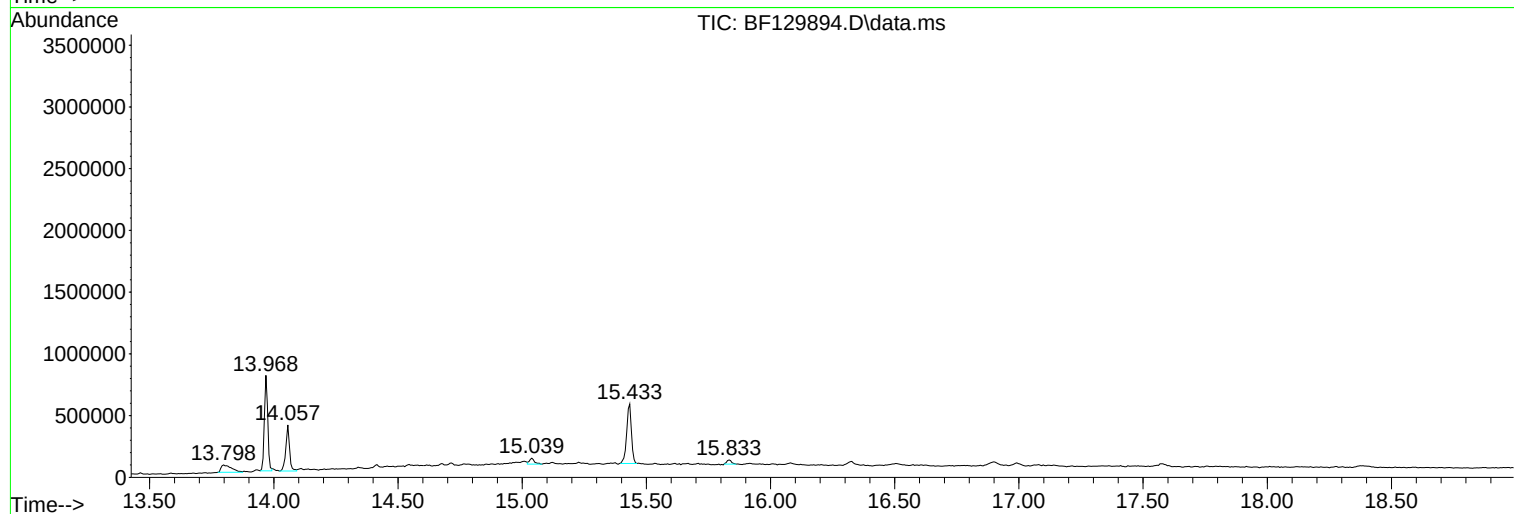
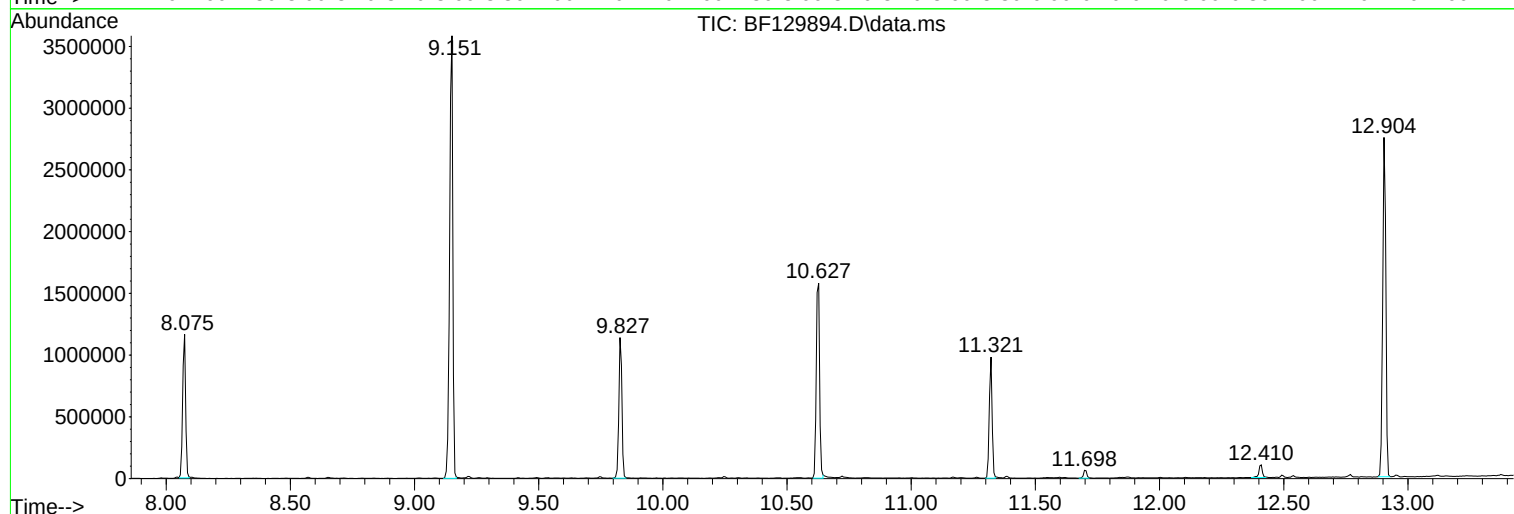
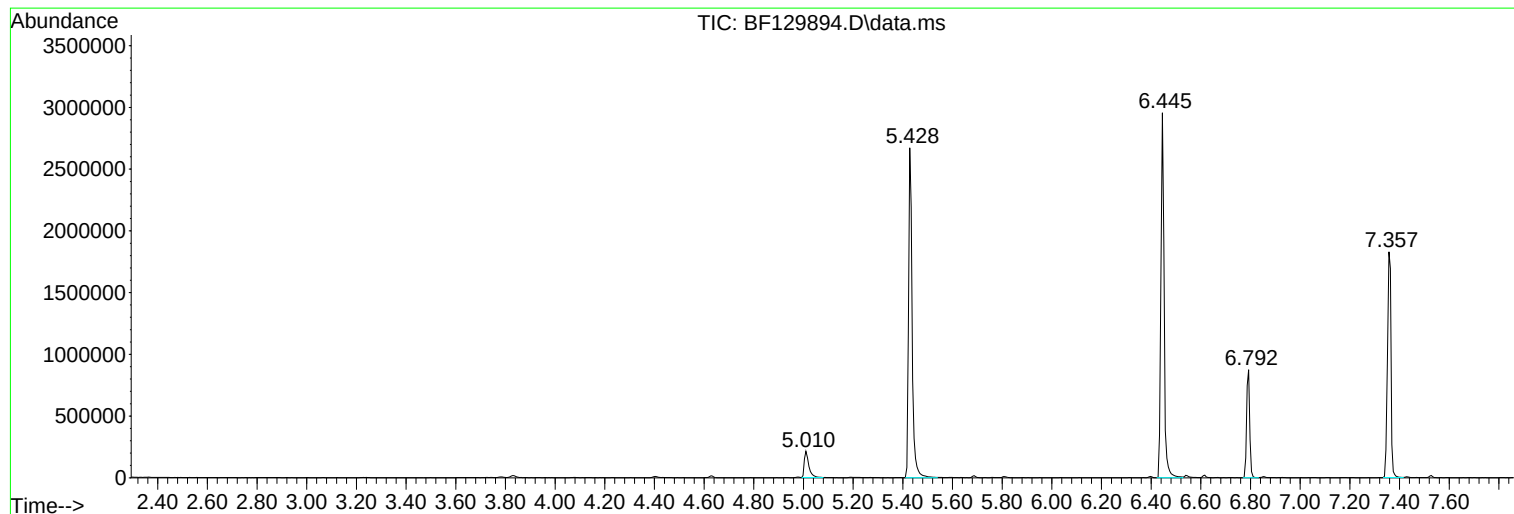
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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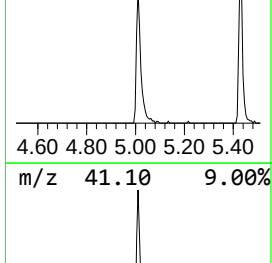
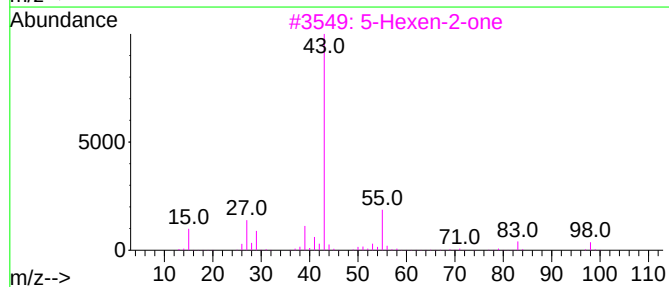
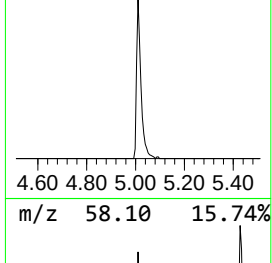
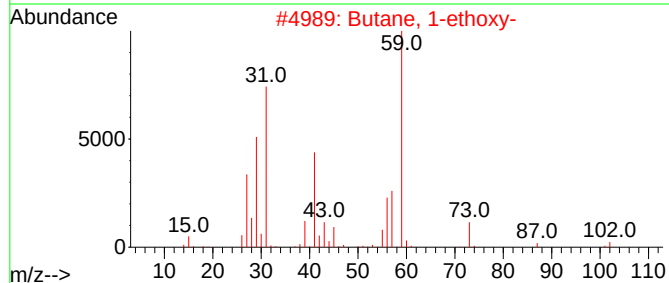
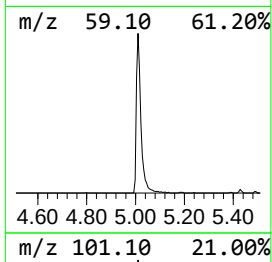
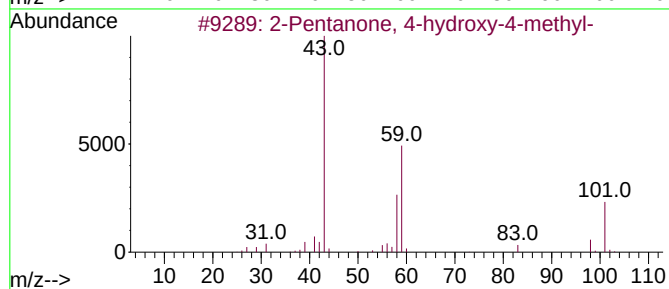
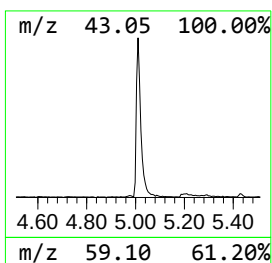
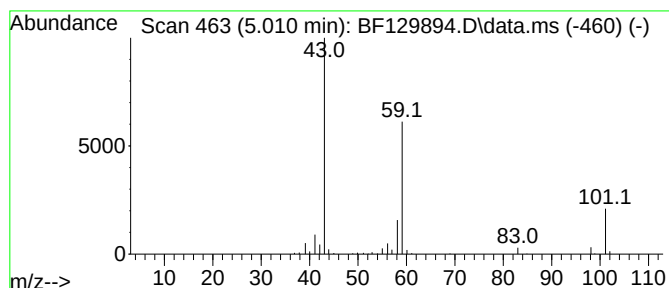
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	7.04 ng	268134	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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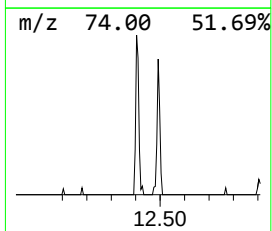
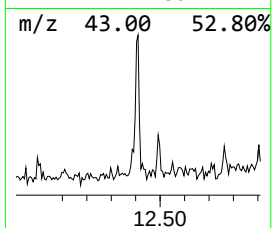
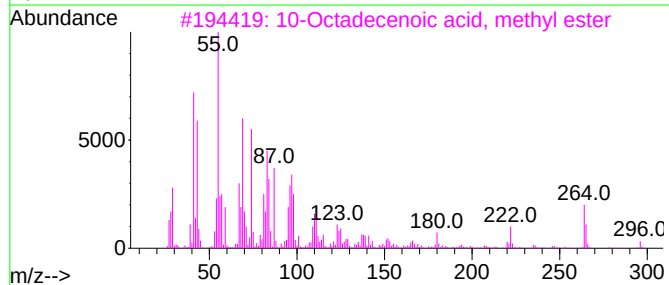
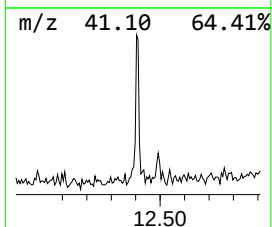
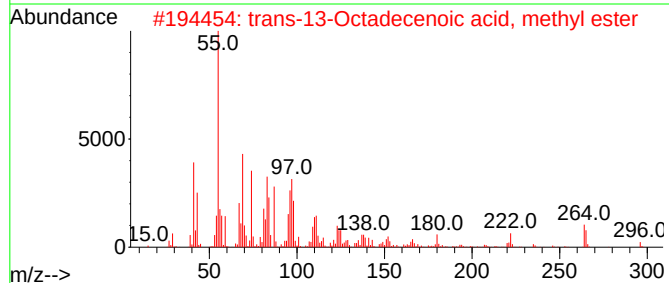
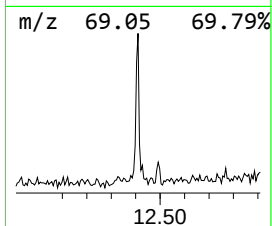
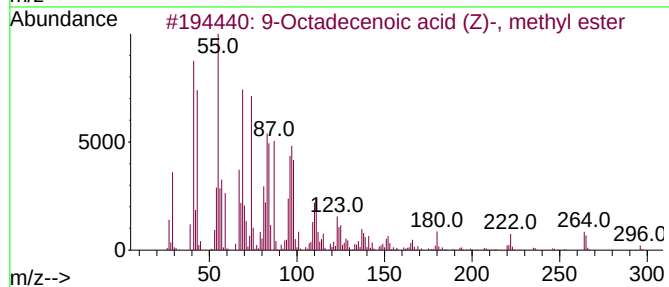
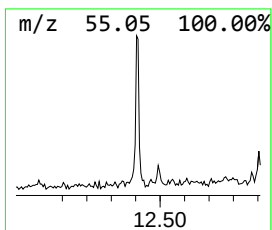
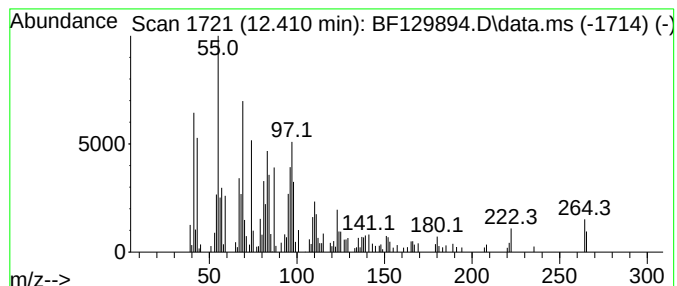
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Peak Number 2 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	2.54 ng	101092	Phenanthrene-d10	11.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
3			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
4			6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	81
5			Methyl myristoleate	240	C15H28O2	056219-06-8	64



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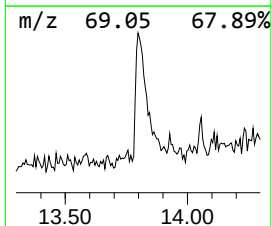
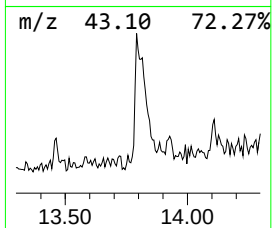
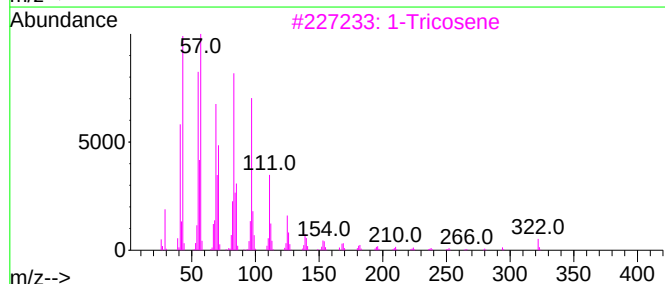
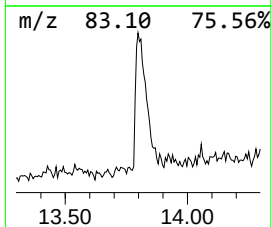
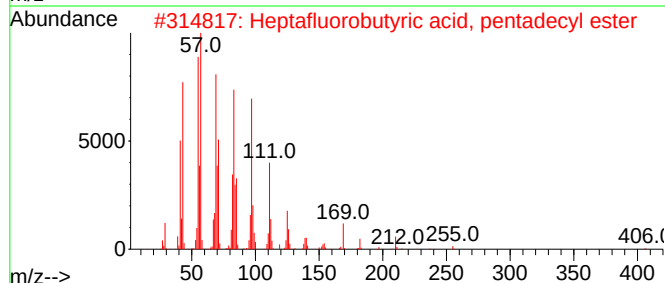
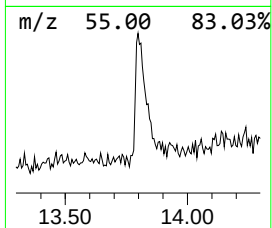
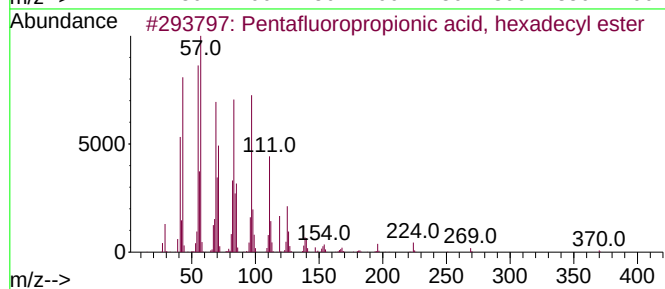
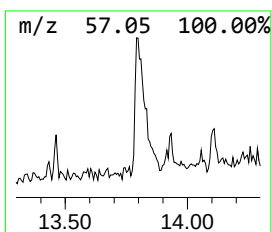
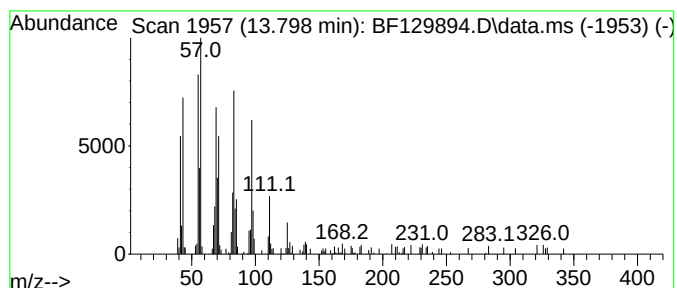
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Peak Number 3 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	4.85 ng	176686	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3			1-Tricosene	322	C23H46	018835-32-0	91
4			Cyclopentadecane	210	C15H30	000295-48-7	89
5			Cyclotetracosane	336	C24H48	000297-03-0	87



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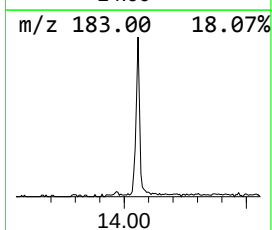
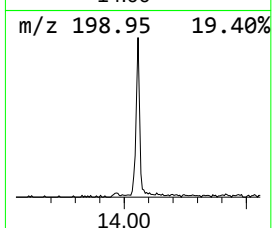
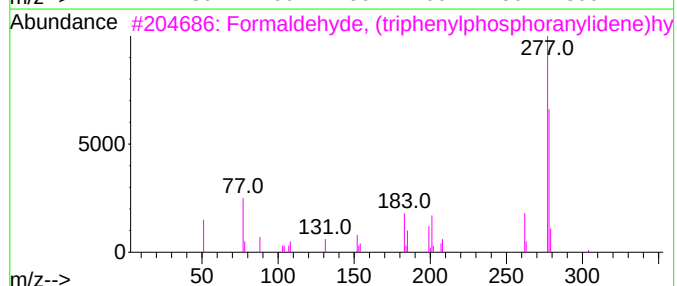
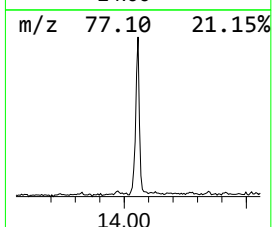
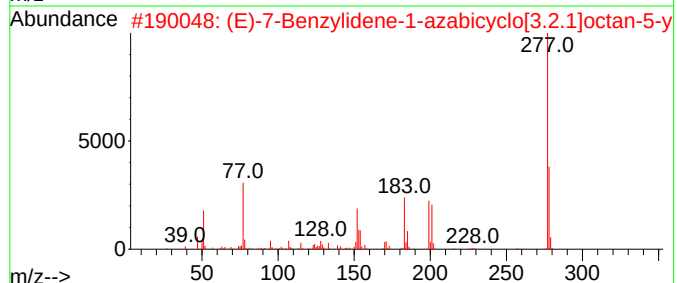
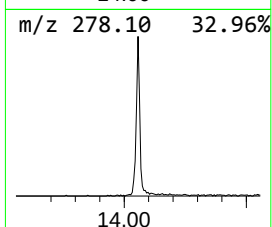
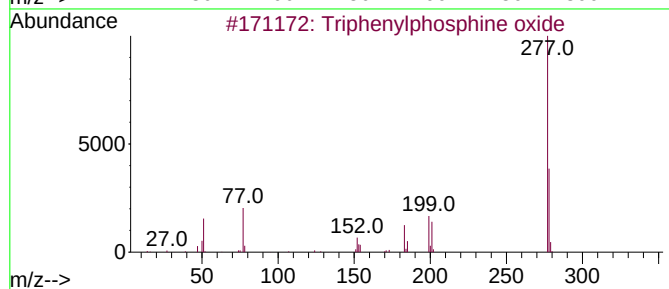
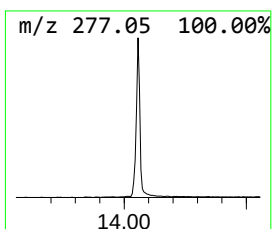
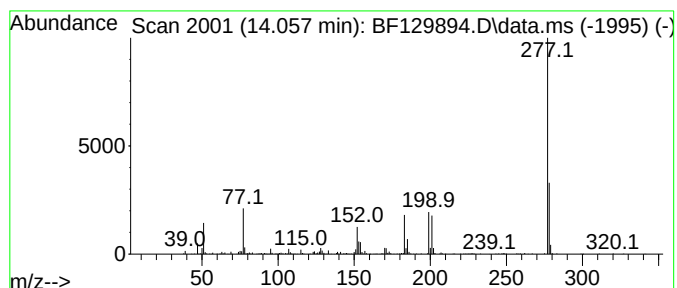
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.057	10.80 ng	393673	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	62
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	45
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32
5			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	32



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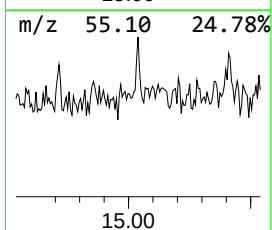
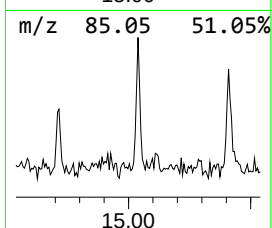
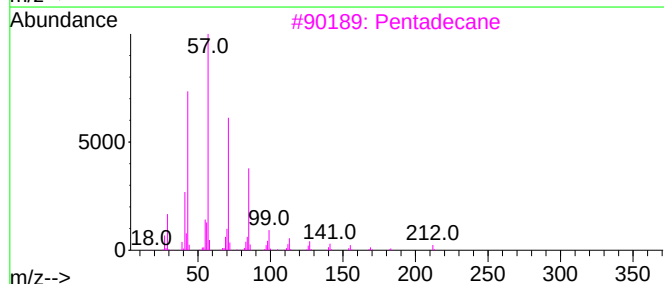
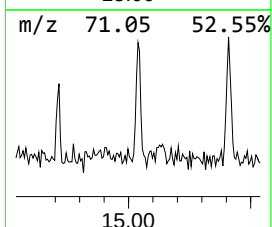
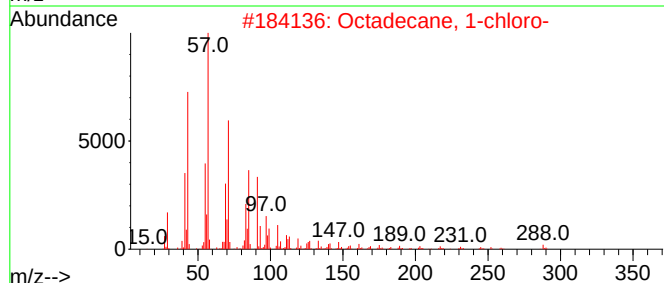
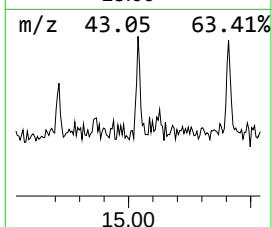
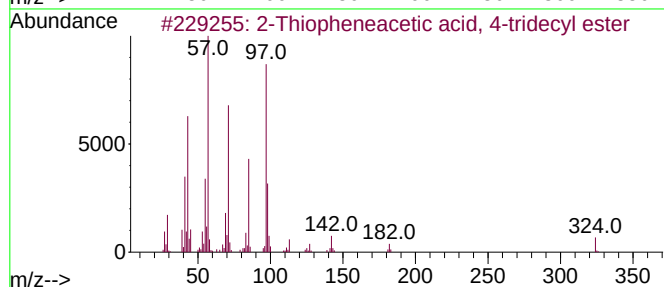
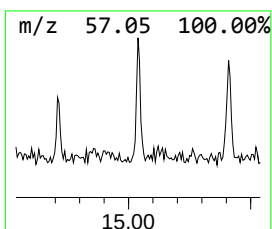
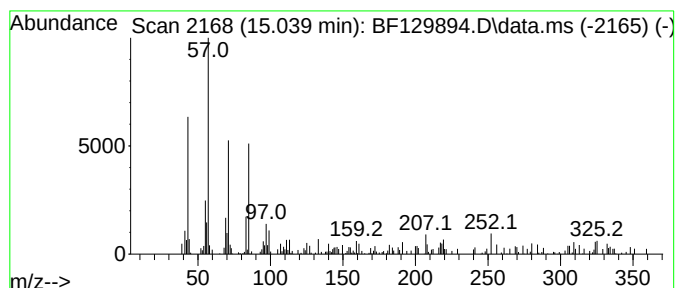
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Peak Number 5 2-Thiopheneacetic acid, 4-t... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.039	2.12 ng	66810	Perylene-d12	15.433

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Thiopheneacetic acid, 4-tridec...	324	C19H32O2S	1000280-66-8	64
2		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	60
3		Pentadecane	212	C15H32	000629-62-9	60
4		Heptadecane	240	C17H36	000629-78-7	53
5		Hentriacontane	437	C31H64	000630-04-6	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.010	7.0	ng	268134	1	6.792	761387	20.0
9-Octadecenoic ...	12.410	2.5	ng	101092	4	11.321	795258	20.0
Pentafluoroprop...	13.798	4.8	ng	176686	5	13.968	729193	20.0
Triphenylphosph...	14.057	10.8	ng	393673	5	13.968	729193	20.0
2-Thiopheneacet...	15.039	2.1	ng	66810	6	15.433	631365	20.0